Resource Summary Report

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BindingDB

RRID:SCR_000390
Type: Tool

Proper Citation

BindingDB (RRID:SCR_000390)

Resource Information

URL: http://www.bindingdb.org

Proper Citation: BindingDB (RRID:SCR_000390)

Description: Web accessible database of data extracted from scientific literature, focusing on proteins that are drug-targets or candidate drug-targets and for which structural data are present in Protein Data Bank . Website supports query types including searches by chemical structure, substructure and similarity, protein sequence, ligand and protein names, affinity ranges and molecular weight . Data sets generated by BindingDB queries can be downloaded in form of annotated SDfiles for further analysis, or used as basis for virtual screening of compound database uploaded by user. Data are linked to structural data in PDB via PDB IDs and chemical and sequence searches, and to literature in PubMed via PubMed IDs .

Synonyms: BindingDB

Resource Type: data or information resource, database

Defining Citation: PMID:26481362, PMID:17145705

Keywords: drug, drug discovery, drug target, binding affinity, protein interaction, small molecule-protein interaction, interaction, protein, small molecule, FASEB list

Funding: NIGMS GM070064;
NSF 9808318;
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Availability: Free, Freely available

Resource Name: BindingDB

Resource ID: SCR_000390

Alternate IDs: nif-0000-02603

Record Creation Time: 20220129T080201+0000

Record Last Update: 20250426T055414+0000

Ratings and Alerts

No rating or validation information has been found for BindingDB.

No alerts have been found for BindingDB.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 41 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

Antolin AA, et al. (2018) Objective, Quantitative, Data-Driven Assessment of Chemical Probes. Cell chemical biology, 25(2), 194.

Yang H, et al. (2018) In Silico Prediction of Chemical Toxicity for Drug Design Using Machine Learning Methods and Structural Alerts. Frontiers in chemistry, 6, 30.

Karimzadeh M, et al. (2018) Aberration hubs in protein interaction networks highlight actionable targets in cancer. Oncotarget, 9(38), 25166.

Wang T, et al. (2018) A Computational Systems Pharmacology Approach to Investigate Molecular Mechanisms of Herbal Formula Tian-Ma-Gou-Teng-Yin for Treatment of Alzheimer's Disease. Frontiers in pharmacology, 9, 668.

Cheng F, et al. (2018) Network-based approach to prediction and population-based validation of in silico drug repurposing. Nature communications, 9(1), 2691.

Lacroix S, et al. (2018) A computationally driven analysis of the polyphenol-protein interactome. Scientific reports, 8(1), 2232.

Huo X, et al. (2018) A Component Formula of Chinese Medicine for Hypercholesterolemia

Based on Virtual Screening and Biology Network. Evidence-based complementary and alternative medicine : eCAM, 2018, 1854972.

Song Z, et al. (2018) Systems Pharmacological Approach to Investigate the Mechanism of Acori Tatarinowii Rhizoma for Alzheimer's Disease. Evidence-based complementary and alternative medicine : eCAM, 2018, 5194016.

Himmelstein DS, et al. (2017) Systematic integration of biomedical knowledge prioritizes drugs for repurposing. eLife, 6.

Baptista SJ, et al. (2017) Novel PARP-1 Inhibitor Scaffolds Disclosed by a Dynamic Structure-Based Pharmacophore Approach. PloS one, 12(1), e0170846.

Shen X, et al. (2017) Elucidation of the Anti-Inflammatory Mechanisms of Bupleuri and Scutellariae Radix Using System Pharmacological Analyses. Mediators of inflammation, 2017, 3709874.

Liu J, et al. (2017) Enhance the performance of current scoring functions with the aid of 3D protein-ligand interaction fingerprints. BMC bioinformatics, 18(1), 343.

Fang J, et al. (2017) AlzhCPI: A knowledge base for predicting chemical-protein interactions towards Alzheimer's disease. PloS one, 12(5), e0178347.

Zheng T, et al. (2017) Designing Dietary Recommendations Using System Level Interactomics Analysis and Network-Based Inference. Frontiers in physiology, 8, 753.

Shang J, et al. (2017) Comparative analyses of structural features and scaffold diversity for purchasable compound libraries. Journal of cheminformatics, 9(1), 25.

Fang J, et al. (2017) Systems Pharmacology-Based Discovery of Natural Products for Precision Oncology Through Targeting Cancer Mutated Genes. CPT: pharmacometrics & systems pharmacology, 6(3), 177.

Suh SY, et al. (2017) Systems Pharmacological Approach of Pulsatillae Radix on Treating Crohn's Disease. Evidence-based complementary and alternative medicine : eCAM, 2017, 4198035.

Gilson MK, et al. (2016) BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology. Nucleic acids research, 44(D1), D1045.

Basse MJ, et al. (2016) 2P2Idb v2: update of a structural database dedicated to orthosteric modulation of protein-protein interactions. Database : the journal of biological databases and curation, 2016.

Zhou B, et al. (2016) Predicting cancer-relevant proteins using an improved molecular similarity ensemble approach. Oncotarget, 7(22), 32394.